Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.55

Global applicability domain: Inside

Local applicability domain index: 6.05e-01

Confidence level: 6.54e-01

Nearest Neighbors from the Training Set

Image not found
1-Ethyl-2-methylbenzene
Measured: 3.53
Predicted: 3.47

Image not found
Cumene
Measured: 3.66
Predicted: 3.77

Image not found
3-Ethyltoluene
Measured: 3.98
Predicted: 3.55

Image not found
3-fluoropropylbenzene
Measured: 2.95
Predicted: 3.43

Image not found
4-Ethyltoluene
Measured: 3.63
Predicted: 3.55